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SYNOPSIS

ON

Studies of Kerr rotations in tilted multi-Weyl semimetals and other gapless systems

For the degree of Doctor Of Philosophy in Physics with permission from the department of physics, faculty of Science L.N.M.U, Darbhanga, 846004

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1 Introduction and Review of Literature

The last decade has witnessed Weyl semimetals (WSMs) as a focus of research attraction due to their exotic properties. It is manifested due to its unusual Fermi arc surface states and chiral anomaly that is intimately related to topology and symmetry of WSMs [1, 2]. In WSMs,the bulk band gap closes at an even number of discrete points in the Brillouin zone(BZ). These special band closing non-generate points are referred as Weyl nodes or points [3]; Weyl nodes act as a monopoles or antimonopoles of Berry curvature characterized by monopole charge J. Two Weyl nodes of different chirality are located at different momenta when the system breaks thet time-reversal symmetry; four Weyl nodes are noticed in general for systems with broken inversion symmetry only [1, 4]. Moreover, inversion breaking may also lead to the energy-separated Weyl points while time-reversal-symmetry breakingcan result in Weyl points at the same energy [5, 6]. The existence of Fermi arc surface states, chiral-anomaly-related negative magnetoresistance, and the quantum anomalous Hall effect is the direct consequence of the nonzero fluxes of the Berry curvature[7, 8, 9]. As compared to the conventional WSMs with n=1, reported in TaP, TaAs, and NbAs [10, 11, 12], it has been recently shown that J can be generically greater than 1, with the crystalline symmetries bounding its maximum value to 3[13, 14, 15]. These are called multi-WSMs (mWSMs). These WSMs can be considered as 3D analog of multilayers graphene [16]. Close to the Weyl points, mWSMs host low-energy quasiparticles with the dispersion which is linear only in one direction and quadratic(cubic) in other two directions leading to usual properties which differ from linear WSMs [17, 18, 19, 20, 21, 22, 23]. From the density functional theory (DFT)calculations, it has been suggested that $HgCr_2Se_4$and $SrSi_2$can be the candidate materials for double WSM [15, 13, 24] whereas $A(MoX)_3$(withA=Rb,TI;X=Te) kind of materials can accommodate triple-Weyl points[25].

Topological Weyl semimetals (TWS) can be classified as type I TWS, in which WSM has a conical spectrum and a point-likeFermi surface at the Weyl point which corresponds the density of states vanishes at the Weyl nodes, and type II TWS(which occurs when large tilting of the Weyl cones results ina Lifshitz transition), in which an electron pocket and a hole pocket meet at a singular point of momentum space, allowing for distinct topological properties [1, 26, 27, 28, 29, 21]. The existence of type-II WSM has been

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experimentally demonstrated [30, 31] while theoretical prediction shows that a type-II WSM can be engineered by applying strain or chemical doping to the original type-I WSM [32]. The type-II WSM phase is characterized by a different class of Weyl fermions manifesting the violation of Lorentz symmetry. Type-II WSMs can yield intriguing electronic transportproperties due to a markedly different density of states atthe Fermi level [33, 34, 35, 36]. While a lot of progress has been made experimentally and theoretically in investigating n=1 type-I and type-II WSMs, the experimental discovery of mWSMs with $n \geq 2$ is yet to be made; however, using density functional theorycalculations some materials are conjectured to host Weyl nodes with monopole charges n=2,3 [13, 15, 24, 25].

Here, we demonstrate the existence of giant polarization rotation in the electrodynamic response in tilted mWSMs with broken time-reversal symmetry. Our results generalize the study of Ref. [[37]] to include topological charge J in type-I and type-II WSMs at finite chemical potential. We analytically and numerically calculate the full complex optical conductivity matrix for tilted type-I and type-II mWSMs including finite chemical potential and the internodal separation. This allows us to obtain the polarization rotation for the thin-film geometry as well as for bulk WSMs. In WSM thin films, the giant Kerr rotation (GKR), polarization rotation in the reflected beam, originates from the optical Hall conductivity including the QAH effect [37]. We analytically as well as numerically calculate the full optical conductivity matrix $\sigma_{ij}(\omega)$ for tilted type-I and type-II mWSMs.

In bulk WSM large optical activity is predominantly caused by the axion electrodynamics induced changes in the Maxwell equations. The effective dielectric constant of the modified Maxwell equation can be expressed as $\epsilon'_{ij} = \epsilon_{ij} + \varepsilon_{ijk} Q_k \times 2i\alpha_F c/\pi\omega$, where the second term establishes Q/ω to be the effective "gyrotropy" constant, analogous to magnetization in magnetic systems. This axion-induced gyrotropy is what leads to optical activity in bulk WSMs, even in the Pauli-blocked regime with forbidden optical transitions. For light incident parallel to the Weyl node separation (on surfaces without Fermi arc states), only circular eigenmodes are allowed in the WSM, leading to large circular birefringence and circular dichroism, along with the giant Kerr effect, which is odd in Q. For light incident on surface perpendicular to the Weyl node separation (on surfaces with Fermi arc states), there is large linear birefringence and dichroism, along with a polarization angle

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dependent giant Kerr effect which is an even function of Q.

2 Objective of proposed work

We will calculate the optical conductivity of type-I and type-II multi-Weyl semimetals(m-WSMs) in time-reversal(TR) broken case at finite doping. It would be interestng to see the behavior of both longitudinal and Hall conductivities on J(monopole number). The Kerr rotations in thin films and bulk have different dependence on system parameters. We would also be interested to see the dependence of Kerr rotation in thin films on monopole charge J and Fermi velocity v_F. We will apply some techniques to calculate the Kerr rotations for other gapless systems such as triple Weyl fermions and nodal line semimetals etc.

3 Plan of work and Methodology

The non-interacting low energy effective Hamiltonian for tilted multi-Weyl semimetals is given by [39, 40, 21, 41],

$$\mathcal{H}_J = \hbar v_t k_z 1_{2\times 2} + \alpha_J \hbar[(\hat{k}_-)^J \sigma_+ + (\hat{k}_+)^J \sigma_-] + \chi \hbar v_z \hat{k}_z \sigma_z, \tag{1}$$

where $\sigma_\pm = \frac{1}{2}(\sigma_x \pm i\sigma_y)$ and $\hat{k}_\pm = \hat{k}_x \pm i\hat{k}_y$, J represents monopole charge, v_z is the effective velocity along $\hat{z}$ direction and α_J is the material dependent parameter, e.g. α_1 and α_2 are the Fermi velocity and inverse of the mass respectively for the isotropic and double WSMs. The energy spectrum of Eq.(1),
To avoid difficulties with anisotropic dispersions, we consider the following coordinate transformation [?]

$$k_x \to \rho^{1/J}\cos\phi, k_y \to \rho^{1/J}\sin\phi, k_z \to k_z \tag{2}$$

whose Jacobian is given by

$$\mathcal{J} = \frac{\rho^{\frac{2}{J}-1}}{J} \equiv \mathcal{J}(\rho) \tag{3}$$

In the transformed coordinates, the energy dispersion is given by $E_s(\mathbf{k}) = \hbar v_t k_z + s\hbar\sqrt{\alpha_n^2(\rho_J)^2 + (k_z v_z)^2}$ with $\rho_J = (k_x^2 + k_y^2)^{J/2}$.

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3.1 Calculation of Kerr rotations

The interband optical conductivity in the non-interacting limit $\gamma \to 0$ can be expressed as

$$\sigma_{\alpha\beta}(\omega) = -\lim_{\gamma\to 0}\sum_{\mathbf{k}} \frac{in_k}{\hbar\omega_k}\frac{M_i^{ss'}(k)M_j^{s's}(k)}{\hbar\omega + \hbar\omega_k + i\gamma} \tag{4}$$

where $i, j = x, y, z, n_k^{eq} = \Theta(\mu - \hbar v_t k_z - \epsilon_J) - \Theta(\mu - \hbar v_t k_z + \epsilon_J)$ and $\hbar\omega_k = 2\hbar\epsilon_j(k)$ is the energy difference between the conduction and the valence band, which is independent of the tilt velocity. The real and the imaginary parts can be separated in the limit $\gamma \to 0$, using the Sokhotski-Plemelj Formula

$$\lim_{\gamma\to 0}\frac{1}{x \pm i\gamma} = P\frac{1}{x} \mp i\pi\delta(x) \tag{5}$$

Here P denotes the principal value.

The optical matrix element is given by

$$\begin{aligned} M_x &= e\alpha_J(i\sin J\phi - \xi\frac{v_F k_z}{\epsilon_J}\cos J\phi), \\ M_y &= e\alpha_J(-i\cos J\phi - \xi\frac{v_F k_z}{\epsilon_J}\sin J\phi) \\ M_z &= \xi e v_F\frac{\alpha_J\rho}{\epsilon_J} \end{aligned} \tag{6}$$

Here we have defined $\epsilon_J = \hbar\sqrt{\alpha_J^2\rho^2 + v_F^2 k_z^2}$. Note that $\mathbf{M_k}$does not depend on the tilt velocity v_t at all.

4 Expected Results

In WSM thin films, the giant Kerr rotation (GKR), polarization rotation in the reflected beam, originates from the optical Hall conductivity including the QAH effect [37]. We would analytically as well as numerically calculate the full optical conductivity matrix $\sigma_{ij}(\omega)$ for tilted type-I and type-II mWSMs. For light incident on the WSM thin film surface without the Fermi arc states (perpendicular to the node separation), the Kerr angle $\Theta_{Kerr} \propto \sigma_{xy}/\sigma_{xx}$ would be independent of monopole charge J. For realistic material parameters, the Kerr angle is found to be of the order of 10^{-1} radians for optical

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frequencies below 10^{14} Hz in the case of single WSM. This is large compared to the usually observed values in topological insulators [38]. For light incident on the surface with Fermi arc states (parallel to the node separation), we find that $\Theta_{Kerr} \propto \sigma_{yz}/\sigma_{zz} = 0$ [37].

In bulk WSM large optical activity is predominantly caused by the axion electrodynamics induced changes in the Maxwell equations. The effective dielectric constant of the modified Maxwell equation can be expressed as $\epsilon'_{ij} = \epsilon_{ij} + \varepsilon_{ijk} Q_k \times 2i\alpha_F c/\pi\omega$, where the second term establishes Q/ω to be the effective "gyrotropy" constant, analogous to magnetization in magnetic systems. This axion-induced gyrotropy is what leads to optical activity in bulk WSMs, even in the Pauli-blocked regime with forbidden optical transitions. For light incident parallel to the Weyl node separation (on surfaces without Fermi arc states), only circular eigenmodes are allowed in the WSM, leading to large circular birefringence and circular dichroism, along with the giant Kerr effect, which is odd in Q. For light incident on surface perpendicular to the Weyl node separation (on surfaces with Fermi arc states), there is large linear birefringence and dichroism, along with a polarization angle dependent giant Kerr effect which is an even function of Q. The above results can be further extended in inversion symmetry breakng multi-WSMs in the next work of this researh program.

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